AOT Accelerator Operations and Technology Division

LA-UR 13-22992

Name: **Petr Anisimov**
Group: **AOT-HPE**
Mentor: **Bruce Carlsten**

Field of Study: **Physics**
Discipline: **Free Electron Lasers**
Appointment: **Director's Postdoc Fellow**
Title: **Hard X-ray FEL Performance with Laser Bunched Beam**

Abstract

Future x-ray FELs, such LANL signature facility MaRIE, are pushed to shorter wavelengths yet are driven by a low energy electron beam in order to reduce costs. This places stringent demands on electron beam emittance and energy spread. Coherent synchrotron radiation (CSR) in bunch compressors and resistive wall wake in the undulator pipe lead to electron beam emittances and energy spread that are too large to satisfy the FEL requirements. A scheme similar to ESASE [A.A. Zholents, Phys. Rev. STAB 8, 040701 (2005)] can be used to simultaneously mitigate the effects of both CSR and resistive wakes. In this scheme, the electron beam is only weakly compressed to a current of ~600 A, compared with currents of 3-5 kA for existing hard x-ray FELs. After this, a laser interacts with the electron beam in a wiggler in order to impose energy modulation on the beam, and then the electron beam passes through a weak chicane that produces current spikes that are much higher than the average current of the beam. The effect of CSR will be significantly reduced in this scheme. In addition, the undulator resistive wake does not have strong short range effects, so it does not "see" the high current spikes, and only interacts with the low average current of the beam. We are conducting start to finish simulations that compare the output of the proposed MaRIE FEL with the MaRIE FEL based on laser bunched beam.

AOT Accelerator Operations & Technology Division

LA-UR 13-22928

Name: **Jeffrey Kolski**
Group: **AOT-OPS**
Mentor : **Thomas Spickermann**
Field of Study: **Physics**
Discipline: **Accelerator Physics**
Appointment: **Postdoc Research Associate**

Title: **Coherent Space Charge Tune Shift Measurements in the Los Alamos Proton Storage Ring**

Abstract

Charged particles in a circular accelerator undergo transverse oscillations (changing position and angle in phase space) with respect to a so-called closed orbit. The number of transverse oscillations a particle undergoes in one revolution around the machine is defined as the betatron tune. The coherent space charge tune shift describes the average frequency shift experienced by particles due to the self-force of the beam and is proportional to the instantaneous beam current. For long beam pulses like the 290 ns long accumulated beam bunch in the Los Alamos Proton Storage Ring, we can observe the change in the coherent space charge tune shift longitudinally along the pulse. We measure an asymmetric betatron tune profile about the bunch center even though the beam current profile is symmetric about the peak intensity. In addition, we observe the coherent space charge tune shift to vary as a function of turn during a store. Quality measurements of the coherent space charge tune shift may provide a unique handle on interesting physics including wake field effects and electron cloud buildup. We digitize the vertical sum and difference signals from a beam position monitor, stack the digitized vector turn-by-turn, and fit the tune for each slice (0.5 ns digitization bin) along the pulse after a single-turn vertical kick. We compare the difference between the measured/fitted tune and the measured bare tune with the theoretical tune shift and infer a charge neutralization, which we relate to the electron cloud density along the pulse and buildup in turn number.

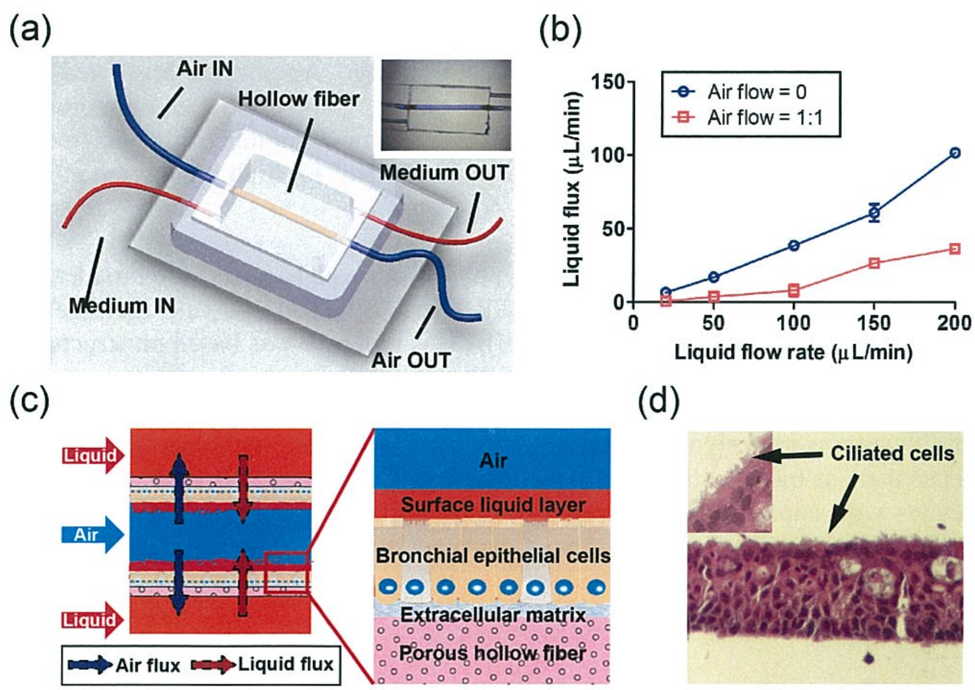
B Bioscience Division

LA-UR 13-22808

Name: **Jen-Huang (Tony) Huang**
Groups: **B-10 and D-3**
Mentors: **Jun Gao and Rashi Iyer**
Field of Study: **Bioscience**
Discipline: **Biomedical Engineering**
Appointment: **Postdoc Research Associate**
Title: **Human Respiratory Lung Bronchioles: In Vitro Bio-Assessment Platform**

Abstract

Development of in vitro human organ bio-assessment platform is essential to replace expensive and time-consuming animal testing models for biomedical research and drug discovery. However, current limitations make it challenging to fabricate accurate, physiologically and functionally relevant human organs. Here, we report a new approach that overcomes these limitations by integrating air-liquid interface using porous hollow fibers to mimic the physiological complexity for the growth of the lung bronchiole compartment. The two phase flow system can simulate a dynamic liquid layer in luminal surface of hollow fiber by alternatively changing air and liquid flow rate. This capability can be harnessed to develop well-differentiated human bronchiolar tissue.



LA-UR 13-23753

Name: **Ramesh Jha**
Groups: **B-10 and B-11**
Mentors: **Charlie Strauss and David Fox**
Field of Study: **Bioscience**
Discipline: **Protein Engineering**
Appointment: **Postdoc Research Associate**
Title: **Transcription Factors Made to Order: Natural or Designed for Synthetic Biology Applications**

Abstract

"Transcription factors" are logic gates at a molecular level in all living systems. They lie at the nexus of detecting an input signal (e.g. a small molecule) and causing a response (triggering production of specific proteins.) For example, if the small molecule represents “food”, the detection event might cause the release of digestive proteins. They do this by acting as gate keepers for the genes they regulate by physically binding the DNA; when a TF protein also binds a small molecule it permits (or denys) access to the specific nearby genes by the cells gene reading machinery.

We are engineering this system to either sense alternative molecules of interest or to produce different molecules in response. In particular a Transcription Factor, called pcaU, from soil bacteria has been transferred to in *E. coli* to detect, 3,4-dihydroxy benzoate (34DHB) of very high commodity value. The TF will cause the bug to produce green fluorescence protein and this allows us to literally see when 34 DHB is present in an individual cell from the green color change. An enzyme borrowed from *Bacillus thuringiensis* allows the cell it is in to produce 34DHB, causing cells to glow green more brightly. We use this engineered ‘biosensor’ to separate high and low efficiency mutants of the enzyme, AsbF at the individual cell level. This will allow us to screen mutants of AsbF for high production efficiency inside the cell.

We have redesigned another Transcription Factor, pobR from soil bacteria, for broadened specificity towards aromatic molecules. The ‘tinkering’ of pobR also resulted in 100-fold increase in sensitivity towards its native inducer, 4-hydroxy benzoate (4HB). This redesign was based on structural homology modeling and docking of the ligand using our Rosetta Structure prediction algorithm.

Our long term objective is to design an array of Transcription Factors with specificity towards custom molecules and use them as biosensors, or tools for evolution of enzymes of interest or for construction of synthetic pathways with applications as green technology, to address energy challenges and alleviate biothreat agents, all consistent with the missions of the laboratory.

B **Bioscience Division**

LA-UR 13-22895

Name: **John Bacik**
Group: **B-11**
Mentor: **Zoe Fisher**
Field of Study: **Bioscience**
Discipline: **Protein Crystallography**
Appointment: **Postdoc Research Associate**
Title: **Structure and Mechanism of Levoglucosan Kinase: Molecular Insights into the Bioconversion of Levoglucosan**

Abstract

Lignocellulosic biomass is an abundant source of carbohydrates that can be used for the production of biofuels. Although inherently robust and resistant to degradation, this material can be effectively broken down through methods of pyrolysis to yield monosaccharide sugars. The necessity for additional processing of biomass-derived sugars arises from the fact that the most abundant sugar product of the pyrolysate is the unusual anhydro-ring containing sugar, levoglucosan (1,6-anhydro-β-D-glucopyranose). Natural bacteria commonly used as biocatalysts such as E. coli lack the ability to metabolize or utilize levoglucosan as a carbon source. However, this sugar can be further enzymatically broken down to glucose-6-phosphate through the activity of the ATP-dependent sugar kinase known as levoglucosan kinase (LGK), which has been isolated from a variety of fungal sources. Genomic integration of recombinant LGK from Lipomyces starkeyi into an engineered ethanologenic E. coli strain has recently been shown to allow for the utilization of levoglucosan as a carbon source for the production of ethanol. In order to gain a better understanding of the mechanism of LGK, we have crystallized and determined several high-resolution X-ray structures of Lipomyces starkeyi LGK. Results from this work have allowed for the unambiguous visualization of reaction substrates and products (levoglucosan, magnesium, manganese, ADP) bound to the enzyme. We are also targeting LGK for neutron crystallography studies, which will reveal the protonation states of key residues and hydrogen bonds in the active site of LGK. The rational design of new LGK constructs and a greater knowledge of factors that contribute to catalytic efficiency will be used to improve applications of this enzyme towards levoglucosan derived biofuel production.

B **Bioscience Division**

LA-UR 13-21797

Name: **Amanda Barry**
Group: **B-11**
Mentor : **Richard Sayre**
Field of Study: **Bioscience**
Discipline: **Bioenergy**
Appointment: **Postdoc Research Associate**

Title: **Determining the Cell Wall Proteome and Engineering Inducible Flocculation in Chlorella sp. for Biofuel Production**

Abstract

In the production of microalgal biofuels, an effective harvesting strategy that results in high biomass yields has yet to be optimized. Currently, microalgal pond biomass represents only ~0.1% of pond volume, and harvesting strategies relying on water removal have high fuel and energy costs. The small particle size and cell density of microalgae is a physical impediment to cell removal. Therefore, a cost-effective strategy to induce microalgae to self-aggregate is desirable. In order to enhance the flocculation of Chlorella protothecoides, a common production strain of microalgae, we are identifying target cell surface proteins by trypsin digestion of whole cells and mass spectrometry (MS) analysis. Unique proteins on the surface of algal cells have been identified for use in tagging of extracellular antibodies. Furthermore, we report the successful transformation of C. protothecoides, and the expression of a novel protein for the production of an aggregating compound that can be extruded from cells for cell flocculation. We describe the construct engineering, transformation, PCR confirmation, mRNA analysis, and compound detection.

C Chemistry Division

LA-UR 13-21774

Name: **Elizabeth (Beth) Judge**
Groups: **C-CDE**
Mentors: **James Barefield**

Field of Study: **Chemistry**
Discipline: **Spectroscopy**
Appointment: **Postdoc Research Associate**
Title: **The Detection and Analysis of Special Nuclear Material in Pellets, Powders, and Ore Form using Laser-induced Breakdown Spectroscopy**

Abstract

Laser-induced breakdown spectroscopy was used to analyze UO_2 / PuO_2 and UO_2 / PuO_2 / AmO_2 / NpO_2 simulated fuel pellets (or mixed actinide oxide samples), depleted uranium and thorium oxide powders and uranium ore as a potential rapid in situ analysis technique in nuclear production facilities, environmental sampling, and in-field forensic applications. This is the first report of the identification and assignments of complex atomic emission spectra of mixed actinide oxides using laser-induced plasma spectroscopy or laser-induced breakdown spectroscopy (LIBS). We have identified and assigned over 800 atomic emission lines for a UO_2 / PuO_2 / AmO_2 / NpO_2 fuel pellet thus far. Material such as pressed pellets and metals, have been extensively studied using LIBS due to the high density of the material and more stable laser-induced plasma formation. Powders, on the other hand, are difficult to analyze using LIBS since ejection and removal of the powder occurs in the laser interaction region. The capability of analyzing powders is important in allowing for rapid analysis of suspicious materials, environmental samples, or trace contamination on surfaces since it most closely represents field samples (soil, small particles, debris etc). The rapid, in situ analysis of samples, including nuclear materials, also reduces costs in sample collection, transportation, sample preparation, and analysis time. Here we demonstrate the detection of actinides in oxide powders and within an uranium ore sample as both pressed pellets and powders on carbon adhesive discs for spectral comparison. Between 5 - 9 mg of powder adhered to each carbon adhesive, with only ~1 μg of material analyzed per laser shot. The acquired LIBS spectra for both forms of the samples differ in overall intensity but yield a similar distribution of atomic emission spectral lines. Finally, we demonstrate that a LIBS system with a resolving power of approximately 20,000 is adequate for analyzing complex mixtures of actinide elements within the same sample.

C **Chemistry Division**

LA-UR 13-22801

Name:	**Kathryn McIntosh**
Group:	**C-CDE**
Mentor :	**George Havrilla**
Field of Study:	**Chemistry**
Discipline:	**Analytical Chemistry**
Appointment:	**Postdoc Research Associate**
Title:	**Microfluidic Sample Preparation for Actinide Characterization by XRF**

Abstract

The accurate determination of plutonium (Pu) in spent nuclear fuel is vital for international safeguards. X-ray fluorescence spectrometry (XRF) is a rapid, nondestructive characterization method well-suited to this application and compatible with other analytical techniques. High resolution x-ray (hiRX) is a monochromatic wavelength dispersive x-ray fluorescence (MWDXRF) method which provides highly selective and sensitive detection of actinides. hiRX uses doubly curved crystal (DCC) optics to produce monochromatic excitation and to collect only a specific characteristic energy (14.279 keV for Pu). In this feasibility study, a prototype microfluidic device or "chip" intended to serve as a sampling system for hiRX was designed and evaluated. The suitability (e.g., chemical resistance and spectral transmission) of several common materials was assessed and the device was constructed using Kapton, polycarbonate, and silicone. A sample chamber with 1 mm diameter was selected to correspond with the excitation spot size of the hiRX, and contains approximately 1 μL of sample when filled with a pipette. Performance of the prototype device was initially evaluated using micro x-ray fluorescence (M-XRF) with aqueous strontium (Sr, a model element for Pu) solutions and spiked synthetic spent fuel (SSF). Between-chip and within-chip repeatability were 5% RSD or less based on net Sr signal intensity in the center of the chamber. A linear response was demonstrated for Sr concentrations up to 0.1%, and future work will evaluate response for Pu in spiked SSF at the 1-2% levels expected in spent fuel. The use of a low-volume sample preparation device which requires minimal sample handling reduces the safety risks associated with analysis of radioactive materials, and is expected to facilitate quantitative determination of Pu with hiRX.

LA-UR 13-22990

Name: **Veronika Mocko**
Groups: **C-CDE and C-IIAC**
Mentors: **Farzaneh Jebrail, Kirk Hollis, and Eva Birnbaum**

Field of Study: **Chemistry**
Discipline: **Chromatography**
Appointment: **Postdoc Research Associate**
Title: **Separation of Ho-163 from Dy Target Material by HPLC**

Abstract

Microcalorimetric determination of neutrino mass requires production of Ho-163 at high rate with high isotopic and chemical purity. There are no fully validated methods for making Ho-163 at the purities and quantities required. Ho-163 will be produced by proton-irradiation of Dy metal target at LANL's Isotope Production Facility. Separation of the desired elemental holmium from parent (target) material dysprosium will be performed by High Performance Liquid Chromatography (HPLC). Preliminary data on the separation of Ho and Dy using natural Ho and Dy are reported herein. Effective and efficient separation of neighboring lanthanides is a challenging task due to similar ionic radii and +III oxidation state. Further difficulty lies in the fact that holmium will be a trace fraction of post-irradiated material. Therefore optimization of the separation is essential to achieve □99% pure holmium fraction. Separation of stable Ho and Dy was performed by HPLC with cation exchange column with alpha-hydroxyisobutyric acid (α-HIB) as eluent and UV-Vis detection using post column reagent PAR (4-(2-pyridylazo)resorcinol). α-HIB is effective chelating agent frequently employed for separation of lanthanides. The effect of HPLC separation parameters such as concentration and pH of the α-HIB on the resolution of Ho and Dy will be discussed.

C **Chemistry Division**

LA-UR 13-23055

Name: **Adam Wachtor**
Groups: **C-CDE and XTD-6**
Mentors: **Farzaneh Jebrail and Robert Gore**

Field of Study: **Physics**
Discipline: **Fluid Dynamics**
Appointment: **Postdoc Research Associate**
Title: **Experimental Investigation of Buoyancy Driven Mixing Due to the Volumetric Energy Deposition of Microwaves**

Abstract

We describe an experiment that seeks to investigate buoyancy driven mixing due to volumetric energy deposition by microwaves. The experiment involves the use of two miscible fluids that are specifically situated such that a light non-polar fluid initially rests on top of a heavier polar fluid – a configuration that is Rayleigh-Taylor stable and if left alone will eventually homogenize due to molecular diffusion. Microwaves are used to preferentially heat the polar fluid, causing its density to eventually drop below that of the non-polar fluid (due to thermal expansion) and creating a Rayleigh-Taylor unstable system for which buoyancy driven mixing will then ensue. We present the evolution of the experimental setup from a proof-of-concept to a customized facility designed for enhanced data collection, describe the parameters that control the time to which the system becomes Rayleigh-Taylor unstable, and interpret the experimental results with the use of theory and modeling.

C **Chemistry Division**

LA-UR 13-22278

Name:	**Matthias Loeble**
Group:	**C-IIAC**
Mentor:	**Stosh Kozimor**
Field of Study:	**Chemistry**
Discipline:	**Inorganic and Actinide Chemistry**
Appointment:	**Postdoc Research Associate**
Title:	**Probing and Quantifying Orbital Mixing in f-Element Molecular Bonding**

Abstract

The covalent sharing of electrons between elements to form chemical bonds represents a fundamental concept in chemistry. Covalency is routinely used to explain reactivity and physical properties across the periodic table. For transition metals, the 3*d*- 4*d*, and 5*d*-orbitals extend well into the periphery of the atom and can interact with valence orbitals of the ligand to form covalent chemical bonds. The situation is more complicated for *f*-elements, and the extent to which these elements participate in covalent bonding remains uncertain.[1] This is especially true for the 5*f*-elements, where decades of study using optical spectroscopy to probe valence 5*f*-orbitals have supported the viewpoint that 5*f*-orbitals are core-like, only weakly perturbed by ligand fields, and not generally involved in covalent bonding. We will present recent efforts in Ligand K edge X-ray absorption spectroscopy (XAS) on the chlorine K edge to assess the roles of n*f* *vs.* (n+1)*d*-orbitals in bonding for *f*-element MCl_6^{n-} compounds in different oxidation states (M = Ce, Nd, Sm, Eu, Gd, U, Pu, n = 1, 2, 3) and show trends how orbital mixing changes going from the 4*f*- to the 5*f*-elements.[2] Next to our well established Cl K edge methodology we will show first examples of our efforts to broaden our spectroscopical portfolio to the metal point of view via complementary spectroscopic techniques, namely high-energy resolution fluorescence detection-XAS (HERFD-XAS) and X-ray emission spectroscopy (XES) in combination with time-dependent density functional theory (TDDFT) and hybrid ground state DFT calculations.

C Chemistry Division

LA-UR 13-22858

Name: **Angela Olson**
Groups: **C-IIAC and C-DO**
Mentors: **Stosh Kozimor and Carol Burns**
Field of Study: **Chemistry**
Discipline: **Inorganic and Actinide Chemistry**
Appointment: **Postdoc Research Associate**
Title: **Orbital Mixing in Dithiophosphinate Actinide Extractants: Advancements in Solution-Phase Sulfur K-Edge X-Ray Absorption Spectroscopy**

Abstract

Nuclear energy is the most viable alternative to fossil fuel combustion until large-scale renewable energy technologies can be implemented. However, use of nuclear energy is limited by the difficulties in remediation, management, and disposal of nuclear waste and the significant hazard posed by the minor actinides present in spent fuel. Efficient separation of trivalent minor actinides from lanthanide ions represents a long-standing challenge because of the similar chemical properties shared by 4*f*- and 5*f*-elements. For reasons not well understood, some soft-donor ligands (e.g., dithiophosphinic acids, R_2PS_2H) are known to selectively extract actinides from lanthanides, with Am/Eu separation factors on the order of 100,000 observed. It is likely that this phenomenon results from increased covalency with actinides over lanthanides; however, a clear understanding of *f*-element participation in covalent bonding has not been established. Recent pioneering work of Solomon, Hedman, and Hodgson significantly advanced capabilities in ligand K-edge X-ray absorption spectroscopy (XAS) to directly measure covalency in bonding. We evaluate $M–S_2PR_2$ orbital mixing in a family of dithiophosphinate extractants by comparing the solid-state and solution-phase sulfur K-edge X-ray absorption spectra, in conjunction with time-dependent density functional theory (TDDFT). The conclusions derived from solid-state S K-edge measurements are validated through comparison with extractants in solution, providing a foundation for *in situ* studies of liquid-liquid extraction systems. Furthermore, we investigate the relative roles of 3*d*, 4*d*, 5*d*, and 6*d*/5*f*-orbitals in M–S covalent bonding and provide preliminary insight into the structure-to-function relationships that may correlate with the selective extraction of trivalent minor actinides from trivalent lanthanides.

C Chemistry Division

LA-UR 13-23001

Name:	**Charles Arnold**
Group:	**C-NR**
Mentors:	**Todd Bredeweg and Marian Jandel**
Field of Study:	**Physics**
Discipline:	**Nuclear Physics**
Appointment:	**Postdoc Research Associate**
Title:	**Refining Radchem Detectors: Iridium**

Abstract

Accurate determination of neutron fluence is an important diagnostic of nuclear device performance, whether the device is a commercial reactor, a critical assembly or an explosive device. One important method for neutron fluence determination, generally referred to as dosimetry, is based on exploiting various threshold reactions of elements such as iridium. It is possible to infer details about the integrated neutron energy spectrum to which the dosimetry sample or "radiochemical detector" was exposed by measuring specific activation products post-irradiation. The ability of radchem detectors like iridium to give accurate neutron fluence measurements is limited by the precision of the cross-sections in the production/destruction network (189lr-193lr). The Detector for Advanced Neutron Capture Experiments (DANCE) located at LANSCE is ideal for refining neutron capture cross sections of iridium isotopes. Recent results from a measurement of neutron capture on 193-lr are promising. Plans to measure other iridium isotopes are underway.

C **Chemistry Division**

LA-UR 12-26052

Name: **Beau Barker**
Groups: **C-NR and MET-1**
Mentors: **Marianne Wilkerson and John Berg**
Field of Study: **Chemistry**
Discipline: **Physical Chemistry**
Appointment: **Seaborg Postdoc Fellow**
Title: **Optically Excited Near-infrared Photoluminescence from NpO22+ in Cs2U(Np)O2C14**

Abstract

Here we present our most recent results on the Cs2NpO2C14 system doped at different concentrations into an isostructural, crystalline uranyl host. Spectra were measured from single crystals of CsNpO2C14 and from crystals of Cs2UO2C14 doped with the neptunyl ion at concentrations ranging from 3% to 50%. The Np near-infrared luminescence is stimulated by excitation of either ligand-to-metal charge-transfer or intra-5f transitions of the Np. There are indications of energy transfer to luminescent excited states of neptunyl following excitation of the uranyl ion in the host crystal. At low Np concentrations, green luminescence typical of uranyl is observed. Increase in Np concentration leads to quenching of the green uranyl emission coincident with stimulation of the Np near-infrared emission. In this presentation, we will describe the observed transitions, as well as decay kinetics and the excitation spectra in the visible and near-infrared spectral regions.

LA-UR 13-21682

Name: **Joanna Denton**
Group: **C-NR**
Mentor: **Michael Murrell**
Field of Study: **Chemistry**
Discipline: **Geochemistry**
Appointment: **Postdoc Research Associate**
Title: **Uranium-Series Environmental Transport and Geochronology Studies**

Abstract

Uranium-series geochemistry and geochronology have a wide range of applications for paleoclimatology, volcanology, environmental risk assessment, and other fields. Recent advances in high-resolution, rapid, in situ microanalytical techniques e.g. LA-ICP-MS and SIMS present numerous opportunities for the geoanalytical community. As with other analytical techniques, the quality of the elemental concentration and isotopic data obtained through microanalytical techniques is dependent on the accurate characterization of suitable reference materials. Even for the case of fs-laser ablation applications, a range of well-characterized standards are required for high precision U-series work. Advances have been made in evaluating existing standard reference materials for U-series isotopic analysis, but this work is ongoing as more reference materials become available.

In this study we present MC-TIMS and MC-ICP-MS results for uranium and thorium isotopic ratios and elemental concentrations measured in a suite of newly available Chinese Geological Standard Glasses (CGSG) designed for microanalysis. These glasses exhibit a range of chemical compositions including basalt, syenite, andesite and a soil. U concentrations for these glasses range from ~2 to 14 ppm and [Th]/[U] ratios range from ~4 to 6. Uranium and thorium concentration and isotopic data will also be presented for a rhyolitic obsidian from Macusani, SE Peru. This obsidian can also be used as a rhyolitic reference material and has a very low Th/U (0.076 atom ratio). Our data on Th and U concentrations are in agreement with prior measurements and provide significantly improved precision. Our data suggest that these standards show a range of disequilibria for 234U/238U (0.93-1.02 activity ratio) and 230Th/238U (0.98-1.12 activity ratio). The disequilibria appear to be primarily due to open system behavior. Characterization of these materials with 238U-234U-230Th disequilibria and extreme Th/U ratios will provide useful reference points for the U-series geoanalytical community.

We are currently developing and evaluating laser ablation methodologies by studying U-series transport and retention in fractures close to natural uranium deposits in Pena Blanca, Mexico. Suitable samples from vertical fractures in the PB-1b core have been identified and preparation is underway for in situ and bulk measurements. Our initial data from these samples indicate that uranium concentrations range from 600 to 5000 ppm and U/Th weight ratios vary from 50 to 600. Some of the U concentrations are nearly as high as in the ore deposit (0.55%). Given the large range in U/Th ratios, construction of whole rock 238U-230Th isochrons should be feasible. Isochron dates will provide information on the timing of U-series mobility in the vertical fractures during the past 350 ka. This work contributes to our understanding of the geochemistry of mineral-water interactions and assessment of radioactive waste repositories, along with other hydrologic and geochemical processes.

LA-UR 13-22999

Name: **Mindy Zimmer**
Group: **C-NR**
Mentors: **Will Kinman and Rob Steiner**
Field of Study: **Chemistry**
Discipline: **Nuclear Forensics**
Appointment: **Postdoc Research Associate**
Title: **Application of the LANL LG-SIMS to Uranium Isotope Analysis of Fallout Debris**

Abstract

Los Alamos National Laboratory recently completed the installation of a Cameca IMS 1280 large geometry secondary ion mass spectrometer (LG-SIMS). The LG-SIMS is capable of providing in situ isotopic and elemental images, and isotopic analyses at high mass resolution (m/Δm 10,000) and high spatial resolution (2 - 250 μm), with a dynamic range of nine orders of magnitude and detection limits in the ppm to ppb range. The LG-SIMS is equipped with both a monocollector and multicollector, with the latter capable of simultaneous detection of up to five species. One challenge of SIMS analysis is finding standards, which must be matrix-matched for quantitative analysis. We will discuss ongoing efforts to develop suitable reference material. The utility of the LG-SIMS will be demonstrated with results of uranium isotope analysis in glassy fallout debris from a historical test. Traditionally, debris analysis is achieved by bulk dissolution, where an entire piece of debris is dissolved. This approach yields the average isotopic composition of the fragment, sacrificing details of small scale heterogeneities, and takes days to weeks to complete. We have analyzed uranium isotopes in 2-4 mm debris fragments from a historical test using both the monocollector and multicollector in a matter of hours. Preliminary results show significant heterogeneity within a single fragment, suggesting that information historically extracted from bulk dissolution of multiple pieces may be revealed in a single piece of debris in as little as a few hours. That such a large amount of information can be extracted from a single fragment in several hours is a remarkable advancement in nuclear forensics, and places LANL at the cutting edge of microanalytical research.

C Chemistry Division

LA-UR 13-25467

Name: **Weon-Kyu Koh**
Group: **C-PCS**
Mentors: **Victor Klimov and Jeff Pietryga**
Field of Study: **Chemistry**
Discipline: **Physical Chemistry, Materials Science, and Nanomaterials**
Appointment: **Postdoc Research Associate**
Title: **Heavily Doped n-Type PbSe and PbS Nanocrystals Using Ground-state Charge Transfer from Cobaltocene**

Abstract

Colloidal nanocrystals (NCs) of lead chalcogenides are a promising class of tunable infrared materials for applications in field-effect transistors (FETs), solar cells, and light emitting diodes. As all of these prospective applications rely on p-n junction architectures, they are greatly hindered by the difficulties in achieving true electronic doping of the NCs, that is, incorporation of charges into the quantum-confined states within the NC core. Reported approaches to NC-doping have utilized incorporation of metal ions, chemical treatments, or electrochemical charge injection, but "heavy doping" of lead chalcogenide NCs, that is, persistent introduction of multiple charges into the quantum-confined band-edge states still represents a significant challenge. Here, we demonstrate that heavily doped n-type PbSe- and PbS NCs can be realized utilizing ground-state electron transfer from molecules of cobaltocene. Using this approach we can inject up to eight electrons per NC into the band-edge 1S state and maintain the high doping level for at least a month even at room temperature. Doping is confirmed by inter- and intra-band optical absorption, as well as by carrier dynamics. Finally, FET measurements of doped NC films and the demonstration of a proof-of-principle p-n diode provide additional pieces of evidence that the developed doping procedure allows for persistent incorporation of electrons into the quantum-confined NC states.

LA-UR 13-20782

Name: **Nikolay Makarov**
Group: **C-PCS**
Mentor: **Victor Klimov**
Field of Study: **Physics**
Discipline: **Ultrafast Spectroscopy**
Appointment: **Director's Postdoc Fellow**
Title: **PbSe/CdSe Core-shell Colloidal Quantum Dots with Enhanced Optical Nonlinearities**

Abstract

Large optical nonlinearities, including two- and three-photon absorption cross sections, nonlinear optical refractive indices, etc. are of immediate interest for various applications including volumetric optical memory, three-dimensional microscopy, optical power limiting, photodynamic therapy, and solar energy conversion. Core-shell colloidal quantum dots are optimal for engineering of large two-photon absorption cross sections due to solution-based processibility of these nanomaterials and fairly straightforward manipulation of optical resonances by varying the dimensions of the core and the shell independently from each other.

Here we present a detailed study of linear and nonlinear optical properties of newly developed PbSe/CdSe core-shell colloidal QDs of various sizes (shell thickness 1-3 nm and core diameter 4-8 nm). One peculiar feature of these QDs is that they exhibit dual emission with one band in the near-infrared (IR) and the other in the visible; these bands originate, from emission of core- and shell-localized charges, respectively. In addition, these novel QDs also show a significant (more than ten-fold) enhancement of two-photon absorption cross sections due to resonant core-mediated transitions and Auger-assisted up-conversion. The latter process is unique to these nanostructures engineered in such a way that the energy released during Auger recombination of a core-localized exciton is sufficient to re-excite a hole from the core to the shell. The enhancement was observed by monitoring visible up-converted emission, excited with the infrared fs laser pulses that are in the range of optical absorption of the PbSe core. Quadratic dependence of the visible emission intensity on excitation power confirms a two-photon excitation mechanism, and the measured cross sections reach ~3x10^7 GM.

Our study demonstrates that the use of core/shell structures represents a promising approach for obtaining enhanced two-photon absorption cross-sections. In addition to traditional applications of two-photon absorption processes, the effect of Auger upconversion can find applications in solar energy conversion for improved harvesting of lower energy IR photons.

C **Chemistry Division**

LA-UR 13-22190

Name:	**Hunter McDaniel**
Group:	**C-PCS**
Mentors:	**Jeff Pietryga and Victor Klimov**
Field of Study:	**Materials Science**
Discipline:	**Photovoltaic Nanomaterials**
Appointment:	**Postdoc Research Associate**
Title:	**Engineered CulnSexS2-x Quantum Dots for High Efficiency Sensitized Solar Cells**

Abstract

In recent years, solar cells incorporating colloidal nanocrystal quantum dots (QDs) as the absorbing material have emerged as leading class of third generation photovoltaics. While the highest efficiencies are somewhat low today (~7%), the rate of improvement is faster than any other type of solar cell technology with a slope of ~1.5%/yr. In collaboration with Sharp Corporation, we are sensitizing meso-porous TiO2 with CuInSexS2-x QDs to fabricate solar cells with an alternative, but still low-cost, device architecture to traditional QD photovoltaics (PVs). With bulk band gaps of 1.0-1.5eV, one of the largest extinction coefficients among direct gap semiconductors, high carrier mobilities, and lack of toxic components, CuInSexS2-x shows great promise as the absorbing component of solar cells. We have shown that gram scale quantities of CuInS2 quantum dots can be synthesized with a range of sizes (and band gaps) with 90%+ chemical yield. More recently, we have modified the synthesis to incorporate controlled amounts of Se to shift the band gap to the near-IR, enabling the capture of more solar photons. By applying mild Cd or Zn treatments to the dots, their photoluminescence (PL) can be enhanced more than 400-fold and the exciton lifetime increases by an order of magnitude without significant changes in absorption. High PL quantum yields imply suppressed non-radiative recombination pathways, crucial for high efficiency PVs. Composition analysis indicates a selective surface-cation exchange gives rise to the enhanced PL by passivation of non-ratiative recombinations sites on QD surfaces. Electron transfer from CuInSexS2-x QDs to meso-porous TiO2 is not significantly hindered by the mild cation-exchange while the increased exciton lifetime results in higher photocurrent and higher voltage. On-going device studies give new insights into strategies for enhancing the performance and durability of QD-sensitized solar cells (QDSSCs), including the importance of reducing recombination pathways such as surface traps without deterring charge transfer. Through optimization of various device elements we have achieved NREL-certified efficiencies exceeding 5% in devices stable for months. While there is significant room for improvement, our result is the highest reported performance and stability for any QDSSC, but unlike most reports, we utilize low-toxicity materials.

C Chemistry Division

LA-UR 13-23067

Name:	**Nicholas Parra-Vasquez**
Groups:	**C-PCS and MPA-CINT**
Mentors:	**Juan Duque and Steve Doorn**
Field of Study:	**Materials Science**
Discipline:	**Spectroscopy and Phase Behavior**
Appointment:	**Director's Postdoc Fellow**
Title:	**Spatially Correlated Photothermal, Fluorescence, and Raman Diffraction-Limited Imaging for Probing Physics at the Nanoscale**

Abstract

In the growing field of mesomaterials, various techniques have been well established to characterize material properties. A great portion of these properties is highly dependent on the nanoscale structure, which may include the addition of nanoparticles. Thus, a better understanding of the nanostructure and the route to create it can lead to discovery of new mesomaterials. Three optical techniques widely used for characterization of materials and nanoparticles are: Fluorescence, Photothermal, and Raman microscopy. Briefly, fluorescence can be used to measure the position of fluorescent nano-objects and can allude to its interactions with the surrounding mesomaterial; photothermal can be used to measure the position of non-fluorescent, absorbing nano-objects and can measure thermal properties of its surrounding mesomaterial; and Raman can be used to measure the position of resonant nano-objects and can indicate anisotropic properties and temperature of the surrounding mesomaterial. We have combined these three optical techniques and superimposed on a diffraction-limited spot to better understand mesomaterial formation and nanostructure. We will start with a model system, focusing on questions proposed about physics at the nanoscale, such as behavior of thermotropic liquid crystalline and polymer phase transitions. We will measure the phase transition dynamics and from the anisotropic optical properties of liquid crystalline molecules, we will extract information on the ordering dynamics during phase formation.

CCS Computer, Computational, and Statistical Sciences Division

LA-UR 13-22750

Name: **Sean Williams**
Group: **CCS-3**
Mentor: **Stephan Eidenbenz**
Field of Study: **Mathematics and Computer Science**
Discipline: **Discrete Event Simulation**
Appointment: **Postdoc Research Associate**
Title: **Themis-1: An Agent-based Model of a Modern Monetary Reserve System**

Abstract

We present Themis, an agent-based simulation of a modern reserve system, along with the financial components of the public sector, and a proxy for the nonbank members of the private sector. The simulation primarily revolves around the key interest rate that benchmarks private lending, which arises from agents' trading within a market for bonds and loans, along with the financial implications of that interest rate. Several tunable parameters allow a user to experiment with different policy configurations and levels of private demand for loans. We both validate the simulation against real-world data, and show the results of three unconventional policy settings: one in which the central bank "loses its appetite" for public debt, a second in which the treasury runs deficits without corresponding debt issuance, and a third in which the central bank uses other policy tools to correct for some of the consequences of the second scenario.

D Defense Systems and Analysis Division

LA-UR 13-23020

Name:	**Reid Priedhorsky**
Group:	**D-4**
Mentor:	**Sara Del Valle**
Field of Study:	**Mathematics and Computer Science**
Discipline:	**Social Computing**
Appointment:	**Postdoc Research Associate**
Title:	**Inferring the Origin Locations of Tweets with Quantitative Confidence**

Abstract

Social Internet content plays an increasingly critical role in many domains, including public health, disaster management, and politics. However, its utility is sharply limited by lack of geographic information; for example, fewer than 1.5% of Twitter messages (tweets) contain a geotag. We propose a scalable, content-based approach to estimate the location of tweets using a novel yet simple variant of gaussian mixture models tuned for this task. Further, given that real-world applications depend on quantified uncertainty of such estimates, we propose novel metrics of accuracy, precision, and calibration, and evaluate our approach accordingly. Experiments on 12 million global, comprehensively multi-lingual tweets show that our approach yields reliable, well-calibrated results competitive with previous computationally intensive methods. Our results also show that a relatively small number of training data are required for good estimates (roughly 25,000 tweets), and trained models are quite time-invariant (effective on tweets many weeks newer than the training set). Finally, we offer an analysis of which types of content provide the most useful location signals.

LA-UR 13-21909

Name: **Allison Aiken**
Groups: **EES-14 and ISR-2**
Mentors: **Manvendra Dubey and Petr Chylek**
Field of Study: **Earth and Space Sciences**
Discipline: **Atmospheric Chemistry**
Appointment: **Director's Postdoc Fellow**
Title: **Black Carbon from Biomass Burning**

Abstract

Approximately 50% of black carbon (BC) aerosols come from wildfires and are estimated to contribute up to ~0.6 W/m2 warming of the atmosphere globally. Organic carbon (OC) from fires condenses and/or mixes with BC resulting in an overall lower forcing of 0.03 ± 0.12 Wm-2 from biomass burning. However, this reduction depends strongly on the composition of the carbonaceous aerosols and on the mixing state of OC and BC. Detailed model treatments and laboratory measurements indicate that a BC core coated with a nonabsorbing OC layer enhances absorption with a positive climate forcing. However, the real-time identification of the coating on this internally mixed BC in the field has only recently become detectable with the analysis of lag times between the scattering and incandescence signals in measurements from the single particle soot photometer (SP2). Direct on-line measurements of BC are made with the SP2, which measures the mass of the particles by incandescence on an individual particle basis, from nearby and aged wildfires in addition to those produced in the laboratory. We investigate BC in concentrated wildfire plumes from the two largest wildfires in New Mexico's history with different ages and compare them to BC from indoor generation from single-source fuels, e.g. ponderosa pine, sampled during the Fire Lab At Missoula Experiments IV (FLAME-IV) at the US Forest Service Rocky Mountain Research Station's Fire Science Laboratory in Missoula, Montana in November of 2012. Plumes from the Las Conchas (LC) Fire, a wildfire that occurred in July-August of 2011 and burned ~157K acres, were sampled in the near-field after only a few hours of aging. Older plumes from the Whitewater Baldy (WB) Fire (May-June, 2012) that burned ~300K acres were sampled from further afield with an aging period of 7-9 hours. FLAME-IV includes real-time sampling from direct emissions, well-mixed samples, and aging studies.

LA-UR 13-23064

Name: **Min Chen**
Group: **EES-14**
Mentors: **Cathy Wilson and Joel Rowland**
Field of Study: **Earth and Space Sciences**
Discipline: **Hydrology**
Appointment: **Postdoc Research Associate**
Title: **Impact of Seasonality, Macro– and micro-Topography on Inundated Area of Arctic Wetland**

Abstract

Wetlands are commonly distributed across the Arctic Coastal Plain of northern Alaska, a low-gradient region underlain by continuous permafrost. They are considered important habitats for the arctic fauna at local scale and important components in the biogeochemical cycle at global scale because of the large carbon stores and potential release of this carbon as CO2 and CH4 due to climate change. These wetlands are recharged seasonally by water from snowmelt and summer rainfall, but their area gradually shrinks during the snow free season every year because of greater evapotranspiration than summer precipitation. How inundated areas change seasonally and what factors drive the spatial distribution of surface waters have not been well explored and quantified. In this study, we used high spatial resolution images WorldView 2 on 4 dates (June 16, 2006, June 24, 2010, July 21, 2010 and August 4, 2010) to investigate the seasonal change and spatial pattern of inundated areas for a 4700 ha wetland near Barrow, AK. We found that the inundated areas decreased dramatically (782 ha, 74%) from June 24 to July 21 and continued to decrease (153 ha, 54%) from July 21 to August 4 in 2010. The total inundated area is negatively correlated to the number of days since snowmelt. In terms of spatial pattern, the inundated area was mainly distributed within drained thaw lake basins. During and right after spring snowmelt, macro-topography controlled the spatial distribution of inundated area. By contrast, in July and August, the micro-topography controlled the distribution of inundated area. In particular, during snowmelt, the drained thaw lake basins with lower elevations tend to have higher percentage of inundated area. In July and August, the drained thaw lake basins with low centered ice-wedge polygons tend to have higher percentage of inundated area. The drained that lake basins with lower elevations and without ice-wedge polygons appear to provide the main drainage pathways through the wetland following snowmelt.

EES Earth and Environmental Sciences Division

LA-UR 13-22852

Name: **Michael Cheshire**
Group: **EES-14**
Mentor: **Florie Caporuscio**
Field of Study: **Earth and Space Sciences**
Discipline: **Mineralogy/Geochemistry**
Appointment: **Postdoc Research Associate**

Title: **Bentonite Clay Evolution at Elevated Pressures and Temperatures: An Experimental Study for Generic Nuclear Repositories**

Abstract

The Used Fuel Disposition campaign is presently engaged in looking at various generic repository options for used fuel disposal. Of interest are the disposal of high heat load canisters (up to 300 C), which may allow for a reduced repository footprint. The focus of this experimental work is to expand our understanding on the bentonite barrier stability under different geochemical, mineralogical, and engineering conditions. Experiments were performed at ~150 bars at temperatures up to 300 C for 4 to 6 weeks. Unprocessed bentonite from Colony, Wyoming was saturated with a K-Ca-Na-Cl-rich water at a 9:1 water:rock ratio. Experiments contained various steel plate or Cu-foils and were buffered along the magnetite-Fe oxygen fugacity univariant line.

The pH, K+, and Ca2+ concentrations dropped, while SiO2(aq), Na+, and SO42- concentrations increased throughout the experiment duration. The alkali and alkaline earth metals aqueous concentrations appear to be buffered via the montmorillonite and clinoptilolite exchange reactions. Mineral alterations were primarily observed during the six week, 300 C experiments. Precursor clinoptilolite underwent extensive recrystallization producing a high-silicon analcime in addition to authigenic silica phases. Pyrite decomposition is first observed ~210 C, producing available H2S to further react with the metal plates or evolve as a gas. There is evidence direct crystallization of fibrous illite occurred during the long-term 300 C conditions. The more notable mineral reactions, however, occurred at the metal/clay interface. Authigenic Fe-saponite and chlorite grew with their basal planes near perpendicular to the steel plate, forming a 10 – 40 µm thick 'corrosion' layer. Partial dissolution of steel plates was the likely iron source for chlorite/saponite formation with the steel plates acting as a growth substrate. System containing copper foils did not evolve H2S(g) due to the crystallization of chalcocite (Cu2S) on the copper surfaces.

Such experiments on representative bentonite-barriers at elevated P, T repository conditions are providing useful information for generic repository studies. It appears that illite or illite/smectite mixed-layer formation is significantly retarded in a closed system due to the Na+ and SiO2(aq) dominated environment and limited K+ supply. Zeolite mineralogy appears to be less stable and undergoes alteration potentially affecting the barrier physical and chemical properties. However, it is unknown to what affect (if any) these mineral alterations will have on the engineered barrier system. This research shows mineral growth on waste container substrates are influenced by the container, buffer, and fluid compositions, in addition to pressure and temperature conditions. The role of these corrosion products on the canister stability canisters at elevated heat loads is currently under investigation.

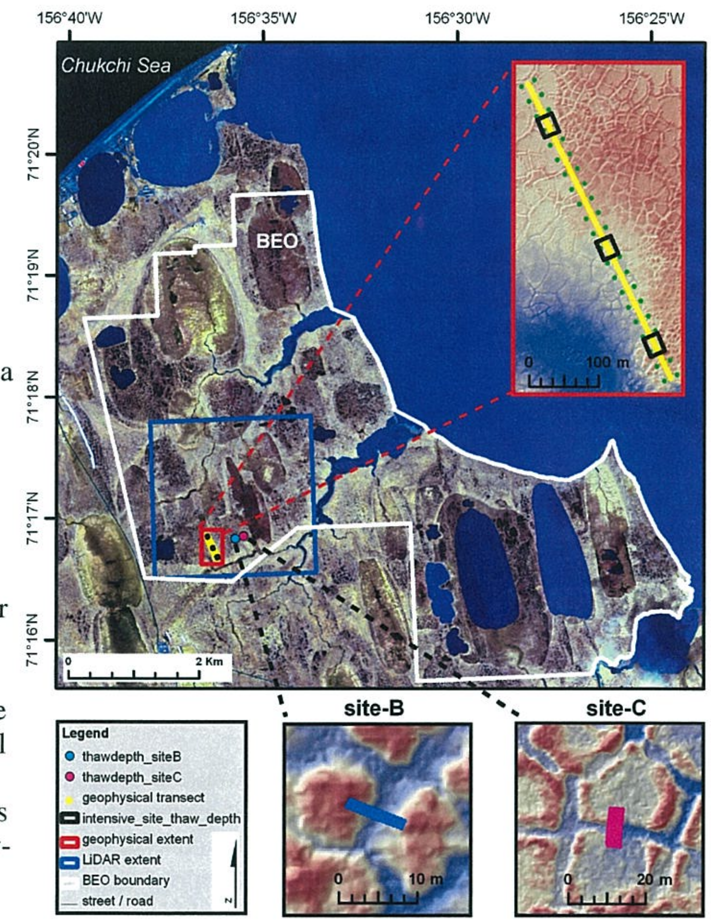
EES Earth and Environmental Sciences Division

LA-UR 13-23231

Name: **Chandana Gangodagamage**
Groups: **EES-14 and ISR-3**
Mentors: **Cathy Wilson and Steven Brumby**
Field of Study: **Earth and Space Sciences**
Discipline: **Civil Engineering/Earth Surface Processes**
Appointment: **Postdoc Research Associate**

Title: **Grand Challenges in Land Surface Characterization: Predicting Earth Surface Processes using High Resolution Remote Sensing Data**

Abstract



What do geospatial patterns on Earth's surface tell us about processes? Do these patterns tell us about underlying processes? Can we use landscape patterns to improve our predictions on the earth surface processes? Earth System Models run at coarse resolutions and the question is how these discretize resolutions represent the surface static and dynamic characteristic. Do our model results agree with the real landscape characteristics? If it does agree, does it just a statistical mean representation or real characterization. Even if it does agree at coarse discretization levels (~ 10-100 km) probabilistically, how do these discretizations represent subgrid scale variability (~ 1 m). How do we scale subgrid scale model variability with the global scale model results or vice versa?

How do Landscape influence/record climate signature? How does our global scale model discretizations represent the landscape climatic signature? Do our global scale models predict the turning point of permafrost thawing into permafrost free condition? How does landscape respond to these changes? When and where do the current continuous permafrost landscape turn into discontinuous or permafrost-free landscapes in next 100 years? Will these landscapes develop a signature more or less like temperate landscapes? Can we unwrap the embedded climatic signature from surface geospatial patterns and fuse it with our global scale model discretization to improve our predictions?

Continued on next page

Los Alamos NATIONAL LABORATORY

EES Earth and Environmental Sciences Division

LA-UR 13-23231

Name: **Chandana Gangodagamage *(continued)***
Groups: **EES-14 and ISR-3**
Mentors: **Cathy Wilson and Steven Brumby**
Field of Study: **Earth and Space Sciences**
Discipline: **Civil Engineering/Earth Surface Processes**
Appointment: **Postdoc Research Associate**
Title: **Grand Challenges in Land Surface Characterization: Predicting Earth Surface Processes using High Resolution Remote Sensing Data**

Abstract

Continued from previous page

Here we provide an example of polygonal ground on the North Slope of Alaska to answer some of the above questions. For terrain with ice-wedge polygons, fine scale characterization is critically important because the processes that govern the carbon cycle and hydrological dynamics are controlled by landscape features on the order of a few to tens of meters. To characterize the polygonal ground in Barrow, Alaska we have combined remotely sensed data from high-resolution LiDAR-derived topography and Worldview 2 satellite imagery with subsurface data derived from geophysics. We use topographic data to develop quantitative metrics that allow for the discretization and characterization of polygons which ultimately define the discretized grid in global scale models.

These metrics include standard topographic variables such as elevation, slope, curvature, and a novel "directed distance" metric. This analysis has allowed us to delineate polygon boundaries, discriminate individual polygon features (rims, troughs, and centers), and broadly classify polygons into types (high versus low). These efforts enable the generation of high resolution modeling grids (pixels ~ 0.25 m) that capture the actual Barrow topography and coarser resolution grids based on a synthetic representation of polygon attributes. In addition to model grid development, we have been able to use distributed measurements of topographic properties and multispectral data to extrapolate point and transect based geophysical data of the subsurface to make landscape-scale predictions of the active layer thicknesses (ALT). Using data fusion approaches, we have successfully developed a methodology for combining topographic metrics with Normalize Difference Vegetation Index (NDVI) and probe measurement of ALT to predict ALT values across our model domain.

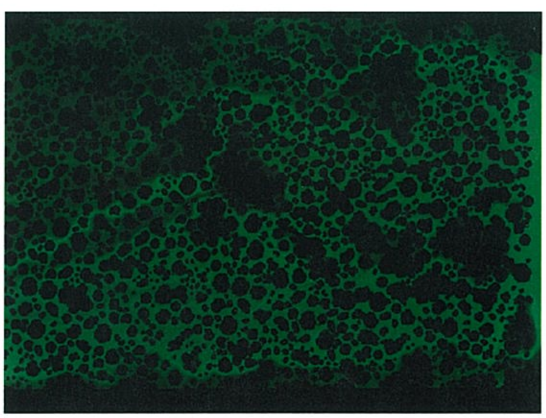
EES Earth and Environmental Sciences Division

LA-UR 13-20819

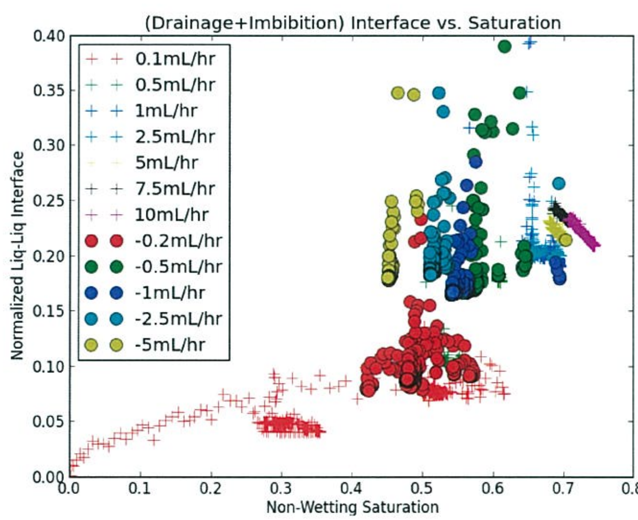
Name: **Peng He**
Group: **EES-14**
Mentors: **Hakim Boukhalfa and Bill Carey**
Field of Study: **Earth and Space Sciences**
Discipline: **Multiphase Flow; Microfluidics**
Appointment: **Postdoc Research Associate**
Title: **Experimental Study of Immiscible Fluid Replacement in a Heterogeneous Microfluidic Pore-Network**

Abstract

Displacement of fluids in porous media is an important process in many energy and environmental applications including remediation of non-aqueous phase liquids (NAPL), geologic sequestration of CO2 in saline aquifers, and enhanced oil recovery. Characterization of fluid displacement processes at the pore scale provides important insights to better understand macroscopic processes and to improve multi-scale computational models. We present here microfluidic experiments of immiscible fluid drainage and imbibitions at ambient conditions using a heterogeneous pore-network that represents a realistic complex geologic medium. The pore network was etched into a silicon wafer with a range of pore-throad sizes from 60 to 800 microns and porosity 0.47. Oil of varying viscosity was used as the wetting fluid and water was used as the non-wetting fluid. Experiments were conducted until steady-state conditions were achieved and quantitative information on flow pattern, interfacial length, and saturation levels were extracted by direct visualization photography) of the experiments. The data demonstrates the significant impact of heterogeneous porosity on capillary trapping and bypass of fluids, which was largely missed in our previous studies performed using homogeneous micromodels. Preliminary results of fluid replacement in pore-network under high-pressure/high-temperature conditions will also be presented.



Fluid Displacement in Heterogeneous Pore-Network



EES Earth and Environmental Sciences Division

LA-UR 13-20532

Name: **Rodica Lindenmaier**

Groups: **EES-14 and ISR-2**

Mentors: **Manvendra Dubey and Brad Henderson**

Field of Study: **Earth and Space Sciences**

Discipline: **Atmospheric Composition**

Appointment: **Postdoc Research Associate**

Title: **Multi-scale CO2 Observations at Four Corners: Seasonal Cycle and Power-plant Signals**

Abstract

There is a pressing need to predict the response of the carbon cycle to climate change as well as verify greenhouse gas emissions from fossil energy sources. To achieve this, we report multi-scale observations of trace gases in the Four Corners, NM region. Ours are the first observations of the carbon cycle in the semi-arid region. The region contains two large coal-fired power plants with real-time in-stack CO2 and pollution monitors, making it an ideal site to evaluate top-down verification methods. We separate the natural column CO2 seasonal variations from the power-plant signals using a variety of methods and determine the seasonal cycle of CO2 to be about 5ppm for 2011 to 2013 and use it to assess GOSAT data.

We have developed a comprehensive test-bed monitoring site near Farmington, NM that includes a solar Fourier Transform Spectrometer (TCCON) and a solar grating spectrometer (Pandora) to monitor column abundance of greenhouse gases (CO2, CH4, N2O) and pollutants (CO and NO2). We also monitor these trace gases and some isotopes (13CO2 and 13CH4) in situ, by cavity ring-down and standard EPA pollution monitors together. We have made continuous measurements for over 16 months. We report the first column regional scale enhancements in CO2 (~ 10 ppm) and NO2 (~ 3 DU) and depleted δ13CO2 (-12 parts per mill) that are attributed to the power plants. These column increases are highly correlated with in situ measurements and the differences can be explained by changes in meteorology. We demonstrate remote observations of columnar NO2/CO2 and δ13CO2 can be used to isolate power-plant sources and constrain emissions. Our study also shows that we can separate the natural carbon cycle from anthropogenic sources and help constrain both of these fluxes.

In 2014 our Solar FTS is scheduled to be deployed in Manaus, Brazil for DOE's GoAmazon project to make the first regional scale measurements of the Amazon carbon cycle and investigate the impacts of the urban plume (nitrogen, ozone, organics) on it.

EES Earth and Environmental Sciences Division

LA-UR 13-22853

Name: **Zewei Quan**
Groups: **EES-14 and MPA-MSID**
Mentors: **Hongwu Xu and Jim Boncella**
Field of Study: **Materials Science**
Discipline: **Semiconductor Nanoparticles**
Appointment: **Oppenheimer Distinguished Postdoc Fellow**
Title: **Investigation of Structural Stability and Assembly Behavior of Lead Chalcogenide Nanoparticles**

Abstract

Lead chalcogenide nanoparticles possess many interesting physical properties such as the relatively larger Bohr exciton radius and smaller band gap, which make them ideal candidates for photovoltaic and thermoelectric applications. However, there are still a lot of things that need to fully be understood such as the stability of these lead chalcogenide nanoparticles, the electron transfer between them with the presence of organic ligands.

I will present how to use the unique in-situ synchrotron high-pressure small angel x-ray scattering (SAXS) and wide angel x-ray scattering (WAXS) technique to investigate the structural stability and assembly behavior of lead chalcogendie nanoparticles. It will include: (1) the first report of reversal Hall-Petch effect of PbTe nanoparticles, (2) the pressure-controlled switches between amorphization and crystallization of PbTe nanoparticles, (3) the formation of stable face-centered-cubic (fcc) superstructures for PbS nanocubes, and (4) the size-dependent final superstructures for PbSe nanoparticles, and the mutual transformation mechanism.

EES **Earth and Environmental Sciences Division**

LA-UR 13-23025

Name: **Heather Throckmorton**
Group: **EES-14**
Mentors: **Jeff Heikoop, Brent D. Newman, and Cathy Wilson**

Field of Study: **Earth and Space Sciences**
Discipline: **Hydrology/Biogeochemistry**
Appointment: **Postdoc Research Associate**
Title: **Isotopic Tracing of Lateral Flows of Water and Carbon in a Permafrost Environment**

Abstract

The Arctic tundra contains a vast amount of C stored in permafrost soils, which are highly susceptible to thawing with climate change. Permafrost degradation has implications for land-atmosphere feedbacks through the release of stored C as greenhouse gases (CO2, methane), and runoff of dissolved C (Guo et al. 2007). Coastal Arctic topography and geomorphology in particular is highly complex, consisting of irregular polygonal ground features, drainage channel networks, and different aged drained thaw lake basins. Such substantial spatial variability complicates predictions of permafrost degradation with regard to land-atmosphere feedbacks affecting climate and regional ecosystem responses. The DOE Office of Science Biological and Environmental Research Program has funded the Next Generation Ecosystem Experiment (NGEE) Arctic project to assess the release of greenhouse gases from melting Arctic permafrost, with emphasis on regional geomorphology; and to establish a coordinated effort among several research institutions to link field observations with process-based models. The role of the research group at LANL is to assess vertical and lateral flows of water and C by collecting field data to validate large-scale regional models.

Waters were collected in August and September of 2012 from the NGEE intensive study sites in the Barrow Environmental Observatory (BEO) in Barrow, Alaska, in two initial synoptic field-sampling surveys. The aims of these field campaigns were to assess geochemical and biogeochemical trends and isotopic variability in waters across unique micro-topographic (polygonal) features and with depth in the active layer above the permafrost. The results will aid interpretation of vertical and lateral C fluxes, and inform future sampling campaigns.

Differences in the concentration of dissolved organic carbon (DOC) occurred with depth and across unique micro-topographic features. Based on the assumption that greater C concentrations indicate a lesser degree of decomposition, results suggest greater decomposition of DOC in surface waters relative to subsurface; and greater decomposition in polygonal troughs and the centers of low-centered polygons, relative to the centers of high-centered polygons and larger drainage networks. The ratio of DOC to dissolved organic nitrogen (DON), as a coarse indicator of decomposition, supported DOC concentrations as an indicator of decomposition, with respect to relative trends with depth and across micro-topographic features. Both DOC concentrations and DOC/DON suggest that less decomposed DOC generally occurred in more saturated (i.e., less oxic) locations, which was not surprising, as these conditions are known to inhibit microbial degradation rates and processes. The stable isotope signatures of 13C-DOC and 15N-DON as decomposition indicators of DOM were not consistent with DOC concentrations or the DOC/DON ratio, despite exhibiting notable variability across water samples. We hypothesize that this discrepancy could be due to unique plant litter inputs within these features, with limited vertical and lateral transport at the study sites. Future work will examine questions addressing these discrepancies, and support and validate models through field observations.

LA-UR 13-23077

Name: **Yassin Labyed**
Group: **EES-17**
Mentor: **Lianjie Huang**
Field of Study: **Engineering**
Discipline: **Medical Imaging**
Appointment: **Postdoc Research Associate**
Title: **Super-resolution Ultrasound Imaging Using a Phase-coherent MUSIC Method with Compensation for the Phase Response of Transducer Elements**

Abstract

Time-reversal imaging with multiple signal classification (TR-MUSIC) can locate pointlike targets beyond the classic resolution limit. In the presence of noise, however, the super-resolution capability of TR-MUSIC is diminished. We develop a new method named the phase-coherent MUSIC (PC-MUSIC) for detecting breast microcalcifications. This algorithm makes use of phase information from multiple frequencies to reduce noise effects and preserve the super resolution. In addition, we account for the phase response of the transducer elements in the derivation of the PC-MUSIC algorithm. However, the phase response of the transducer elements may not be known beforehand. We develop an experimental method to estimate this response using measured signals scattered from a glass micro-sphere embedded in a tissue-mimicking phantom with a homogeneous background medium of a known sound speed. We use numerical simulations to illustrate that the maximum resolution achieved with PC-MUSIC is limited by the transducer bandwidth and the signal-to-noise ratio. We perform experiments on tissue mimicking phantoms and compare images obtained with different imaging modalities, including X-ray mammography, synthetic-aperture ultrasound imaging, TR-MUSIC, and our PC-MUSIC with compensation for the phase response of transducer elements. We demonstrate the significantly improved resolving power of our novel PC-MUSIC imaging and the potential for detecting breast microcalcifications in the clinic.

EES **Earth and Environmental Sciences Division**

LA-UR 13-23066

Name:	**Youzuo Lin**
Group:	**EES-17**
Mentor:	**Lianjie Huang**
Field of Study:	**Bioscience**
Discipline:	**Applied Live Sciences**
Appointment:	**Postdoc Research Associate**
Title:	**Breast Ultrasound-waveforms Tomography with a Modified Total-Variation Regularization Scheme**

Abstract

Early detection of breast cancer is the key to reducing the cancer mortality rate. High-resolution ultrasound waveform tomography has great potential to reliably detect and characterize small breast cancers. Ultrasound waveform tomography is usually ill-posed and requires certain regularization schemes to stabilize the tomography inversion algorithms. We develop a new ultrasound waveform tomography method using a modified total-variation regularization scheme for detecting and characterizing small breast tumors. We employ an alternating-minimization algorithm to efficiently solve the optimization problem. We use numerical breast-phantom data to demonstrate the improved capability of our new tomography method for accurately reconstructs the sound-speed values and shapes of small breast tumors.

LA-UR 13-20178

Name: **Jonathan MacCarthy**
Group: **EES-17**
Mentor: **Dale Anderson**
Field of Study: **Earth and Space Sciences**
Discipline: **Geophysics**
Appointment: **Postdoc Research Associate**
Title: **Combined Rayleigh– and Love-wave Magnitudes for Seismic Event Discrimination and Screening Analysis**

Abstract

The physical basis for the teleseismic Ms:mb seismic discriminant is well-established for Rayleigh waves, but it has also been noted that, for a given mb, shallow earthquake populations typically have larger Love-wave magnitudes than Rayleigh-wave magnitudes compared to explosion populations. The converse is also typically true, suggesting some discrimination potential in Love wave magnitudes. We develop a simple calibrated mathematical formulation for an explosion discriminant that combines Ms (VMAX) Rayleigh- and Love-wave magnitude values, and employs an error model that correctly accounts for estimated variances among events and among stations separately. Error parameters are calibrated using a global data set of Rayleigh-, Love-, and body-wave station magnitudes from 124 earthquakes and 26 nuclear explosions. The calibrated test statistic is applied to the announced May 2009 Democratic Republic of North Korea nuclear test, resulting in a p-value of 0.026 and decision of "reject the null hypothesis: explosion characteristics" at 95% confidence. However, results are compared to an analogous treatment using Rayleigh–only data and calibrations, and demonstrate comparable to improved discrimination performance in the combined Rayleigh + Love case.

EES Earth and Environmental Sciences Division

LA-UR 13-23002

Name: **Sirui Tan**
Group: **EES-17**
Mentor: **Lianjie Huang**
Field of Study: **Earth and Space Sciences**
Discipline: **Geophysics**
Appointment: **Postdoc Research Associate**
Title: **High-Resolution Imaging of Complex Structures using Least-Squares Reverse-Time Migration**

Abstract

Subsurface imaging is a critically important tool for many emerging national energy problems. It can provide crucial information for exploration of Earth's energy resources and for reservoir monitoring. We develop a three-dimensional least-squares reverse-time migration method for cost-effective, high-resolution subsurface imaging of complex structures. Conventional reverse-time migration of limited data suffers from significant image artifacts and low image resolution. Least-squares reverse-time migration iteratively migrates seismic data to reduce image artifacts and improve the image resolution. We apply our method to both synthetic and field data to demonstrate the significant improvement of least-squares reverse-time migration. Least-squares reverse-time migration increases lateral imaging regions and enhances the images of steeply-dipping fault zones that are poorly imaged using conventional reverse-time migration.

ISR **Intelligence and Space Research Division**

LA-UR 13-23188

Name: **John Leacock**
Group: **ISR-1**
Mentors: **Benjamin Norman and Shawn Tornga**
Field of Study: **Physics**
Discipline: **Neutron Lifetime**
Appointment: **Postdoc Research Associate**
Title: **Measuring the Neutron Lifetime in Low Earth Orbit**

Abstract

Neutron lifetime measurements have recently become the subject of excitement within the neutron science community. Several unexpectedly low measurements have forced the Particle Data Group to revise their average value for the neutron mean life from 885.7+/-0.8 seconds in 2010 to 880.1+/-1.1 seconds in 2012.

Current techniques for measuring the neutron lifetime are not statistically limited. The cause for the disagreement is likely due to the uncertainties associated with the systematic corrections of the measurements. A measurement of the neutron lifetime that includes a different set of systematics would therefore be a highly valued contribution to the determination. LANL is uniquely positioned to provide such a measurement.

Neutrons are produced in the atmosphere due to cosmic-ray spallation. Low energy neutrons (<0.65 eV), having been moderated by the atmosphere, are trapped by the gravitational field of the earth. Ignoring neutron decay, the flux of gravitationally bound up- and down-going neutrons would be the same. Because the round trip time for low energy neutrons in LEO (˜500 km) is approximately equal to the lifetime of the neutron, a difference between the up- and down-going fluxes is a measure of neutron decay. A measurement of the up- and down-going neutron fluxes in LEO can provide a systematically different and statistically competitive measurement of the neutron lifetime with a year in orbit.

The methodology of the proposed measurement and a survey of its systematic corrections and uncertainties will be presented.

ISR Intelligence and Space Research Division

LA-UR 13-20735

Name: **Michael Shoemaker**
Group: **ISR-1**
Mentor: **Josef Koller**
Field of Study: **Engineering**
Discipline: **Aerospace Engineering**
Appointment: **Postdoc Research Associate**
Title: **Atmospheric Density Reconstruction Using Satellite Orbit Tomography**

Abstract

Inaccurate atmospheric drag models are the largest remaining error source affecting orbit prediction accuracy for most low-Earth orbit satellites. Error in the modeled atmospheric density is a major contributing factor. Several authors have noted that little progress had been made in reducing the errors in modeled density from the 1960s until recently, during which time errors of 15% or more were common. Drag models errors of this magnitude can result in predicted satellite position errors on the order of 1 km or more after a single day. There has thus been much research attention in recent years on further improving density modeling for drag estimation.

The contribution of this research is the description of a new method, inspired by tomography, to correct atmospheric density models. Tomography is an inverse problem, with various applications in science and engineering, involving the inference of the properties of the material within a body using only measurements taken external to the body. A good example is X-ray computed tomography widely used in medical imaging. Here, X-rays with known intensities are emitted at various angles through a patient's body, where the final intensities of the rays are measured at a detector on the opposite side of the body.

This research describes a new method to estimate the density using a tomography-based approach, where the orbit states of satellites serve as the measurements. The variational equation for the semimajor axis due to perturbing drag acceleration is used to relate the change in osculating specific mechanical energy of the orbit to the integrated density over the orbit. Using several such measurements from a number of satellites, one can estimate the density scale factor (i.e. a correction to an assumed density model). The problem considered here uses measurements from 100 satellites and solves for the spatially resolved global density scale factor discretized over 324 grid elements spanning 300 to 500 km altitude. This ill-posed problem is solved using Tikhonov regularization, with the 3D gradient chosen as the regularization operator, resulting in a penalty on the spatial smoothness of the estimated density. Preliminary simulation results show that the true time-averaged density can be reconstructed to within approximately 10%, using only simulated ground-based tracking measurements separated over 5 orbital revolutions.

ISR Intelligence and Space Research Division

LA-UR 13-23038

Name: **Weichao Tu**
Group: **ISR-1**
Mentor: **Gregory Cunningham**
Field of Study: **Earth and Space Sciences**
Discipline: **Space Science**
Appointment: **Postdoc Research Associate**
Title: **Modeling the Remarkable Enhancement of Killer Electrons in Earth's Outer Radiation Belt with LANL 3D Diffusion Model**

Abstract

The Earth's outer radiation belt consists of MeV electrons and is characterized by large variations in electron flux. Since the MeV 'killer' electrons in the radiation belt can pose a significant threat to space systems, to reliably model and predict their variations is extremely important. The recent success of Van Allen Probes mission has provided us unprecedentedly clean and complete observations of particles and waves in this area. One of the remarkable events captured by the Van Allen Probes mission is the October 8-9 2012 geomagnetic storm event, in which the energetic electron flux in the heart of the outer radiation belt are first wiped out, then exhibit a three-orders-of-magnitude increase on the timescale of hours. Here we simulate this event with our LANL 3D diffusion model to seek the physical explanation for the significant flux enhancement. Our 3D diffusion model includes radial, pitch angle, and momentum diffusion and mixed pitch angle/momentum diffusion driven by wave-particle interactions in the radiation belts. For this event, we use the statistical wave databases based on the CRRES data to derive the diffusion coefficients of plasmaspheric hiss, lower-band and upper-band chorus waves. The outer boundary condition of the model at L*=6 (L* is approximately the radial distance in Earth radii at the equator) is directly derived from the LANL geosynchronous energetic particle data. Another important boundary condition, the low-energy electron source population at 100s of keV, which was usually set to constant, is now made realistic and time-dependent using the newly available MagEIS data from the Van Allen Probes mission. With these data-driven boundary conditions and diffusion coefficients, we can test if the fast and significant increase of MeV electrons observed during the event is produced by energy diffusion from the low-energy source population through interaction with chorus waves, what is the importance of realistic electron source population in this heating process, and meanwhile, what is the role of radial diffusion in accelerating and transporting radiation belt electrons.

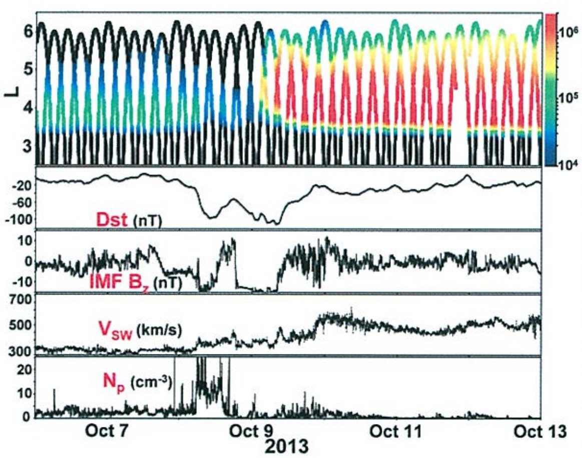


Figure. Top panel shows the 1.8 MeV electron flux measured by the Van Allen Probes mission distributed over time during the October 2012 event and L (approximately the radial distance in Earth radii at the equator). The bottom panels show the geomagnetic index (Dst) and solar wind conditions (IMF Bz, V, and Np) during the event.

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ISR **Intelligence and Space Research Division**

LA-UR 13-22930

Name: **Andrew Walker**
Group: **ISR-1**
Mentor: **Josef Koller**
Field of Study: **Engineering**
Discipline: **Aerospace Engineering**
Appointment: **Postdoc Research Associate**

Title: **Atmospheric and Space Weather Effect on Satellite Drag Coefficients**

Abstract

Inferring atmospheric mass densities from the orbital decay satellites using fixed drag coefficients has introduced biases into empirical atmospheric models. Physical modeling of satellite drag coefficients which simulates the exchange of momentum and energy between the atmospheric gas and the satellite surface can reduce these biases. Physical modeling can be accomplished with closed-form solutions for simple geometries and with either test particle methods or Direct Simulation Monte Carlo for complex geometries. The key unknown in drag coefficient models is the gas-surface interaction which determines the velocity distribution of reflected molecules. The gas-surface interaction model is strongly dependent on the state of the surface (i.e. roughness, adsorpates, etc.); however, observations and measurements of the state of satellite surfaces are sparse and are generally inferred from the orbital decay of spherical satellites or the dynamics of paddlewheel satellites. The effect of atmospheric models and space weather on satellite drag coefficients using the Cercignani-Lampis-Lord (CLL) gas-surface interaction model are investigated. Two other commonly used gas-surface interaction models are also compared to the CLL model: diffuse reflection with incomplete accommodation and Maxwell's model. Maxwell's model is shown incapable of matching the trend of drag coefficients fitted to spherical satellites whereas diffuse reflection with incomplete accommodation closely matches the CLL model. Comparison between the semi-empirical NRLMSISE-00 atmospheric model and the physics-based GITM model shows differences of only a few percent between drag coefficients computed using their respective atmospheric properties during solar maximum. However, at solar minimum the two atmospheric models diverge leading to differences in the computed drag coefficients up to ~10%. Further comparison between drag coefficients computed using GITM atmospheric properties at solar minimum and solar maximum shows differences up to ~25%.

ISR **Intelligence and Space Research Division**

LA-UR 13-22881

Name: **David Graff**
Group: **ISR-2**
Mentor: **Steven Love**
Field of Study: **Physics**
Discipline: **Atomic, Molecular and Optical/Remote Sensing**
Appointment: **Postdoc Research Associate**
Title: **Real-time Matched-filter Imaging for Chemical Detection using a Micro-mirror-based Programmable Filter**

Abstract

Hyperspectral imaging sensors have proven to be powerful tools for highly selective and sensitive chemical detection applications, but have some significant operational drawbacks including a detection time-lag due to the large computational overhead of the matched filter analysis of the resulting data cubes. Spatial light modulation technologies, such as micro-mirror and micro-shutter arrays, and LCD polarization devices, have opened an exciting new arena in spectral imaging: rapidly reprogrammable, high spectral resolution, multi-band spectral filters that perform spectral processing directly in the optical hardware. Our recently developed programmable spectral filter is based on DLP digital micro-mirror device (DMD) technology and mimics a conventional band-pass filter by operating on the spectrum without disturbing the underlying image. With this new technology, even very complicated hyperspectral matched filters can be implemented directly into the optical train of the sensor, producing an image highlighting the target chemical within a spectrally cluttered scene in real-time without further processing. Examples of matched-filter images recorded with our visible-spectrum prototype will be shown, and extensions to other spectral regions such as the "fingerprint regions" of the infrared will be discussed.

ISR Intelligence and Space Research Division

LA-UR 13-22978

Name: **Nina Lanza**
Groups: **ISR– 2 and C-PCS**
Mentors: **Roger Wiens and Sam Clegg**

Field of Study: **Earth and Space Science**
Discipline: **Planetary Science**
Appointment: **Postdoc Research Associate**
Title: **Trends in Rock Surface Compositions on Earth and Mars as Measured by ChemCam**

Abstract

The ChemCam instrument onboard the Mars Science Laboratory 'Curiosity' rover represents the first laser-induced breakdown spectroscopy (LIBS) instrument for extraterrestrial applications. The LIBS technique uses a pulsed laser to ablate small amounts of material from a target to form a plasma. Photons emitted from this plasma are collected by a telescope and directed to three spectrometers covering the UV, VIS, and VNIR. In this way, the ChemCam LIBS instrument may obtain the chemical composition of a target. Because some material is removed during each laser pulse, it is possible to obtain a depth profile of chemical composition by performing multiple laser pulses on one location. Each pulse returns a spectrum that represents the composition at a specific depth, with each subsequent shot sampling the composition at a slightly greater depth. Although the amount of material ablated by each shot varies by material, laboratory measurements of basalts have shown that each LIBS shot removes at least ~0.33-0.5 μm per shot, suggesting a removal of as much as ~25 μm of the surface for 50 shots.

ChemCam's depth profiling capability is significant because the surface chemistry of rocks has the potential to provide significant amounts of information about the history of chemical alteration in a region. Surface coatings are pasted-on layers of material that may not be genetically related to the host rock, while rinds are regions from which particular cations and/or materials have been removed. Both coatings and rinds are often indicative of the past presence of water. On Earth, coatings and rinds may develop even in very arid environments through interactions between the rock surface, airborne dust, and moisture in the atmosphere. The composition and thickness of coatings and rinds provide information about the style of chemical alteration (and amount of water) to which the rock has been exposed. As such, the observation of coatings or rinds on Mars could provide information about both the climate and the presence and abundance of water in the surface environment.

Here we present data from ChemCam's first 100 sols on Mars and compare these to laboratory LIBS experiments on well-characterized terrestrial rock samples with surface coatings and rinds. Initial results from Mars show that almost every rock surface changes from one composition to another within the first ~5 shots, after which the individual rock compositions become distinct from one another. The compositions of the first shots are similar to one another, suggesting a common source. From images it is apparent that rock surfaces contain variable amounts of airfall dust, which likely has a reasonably homogeneous composition. Although most if not all of the compositional changes observed in the first few shots of martian rocks is likely due to dust, it is important to be able to recognize what the signatures of coatings and rinds are in LIBS data. To this end, we have performed a series of laboratory experiments on terrestrial rock samples to compare with martian data in order to better interpret the data being returned from ChemCam; results are forthcoming.

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ISR Intelligence and Space Research Division

LA-UR 13-23841

Name: **Daniela Moody**
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Mentors: **David Smith and Timothy Hamlin**

Field of Study: **Earth and Space Sciences**
Discipline: **Remote Sensing**
Appointment: **Postdoc Research Associate**
Title: **Adaptive Sparse Signal Processing of On-Orbit Lightning Data using Learned Dictionaries**

Abstract

For the past two decades, there has been an ongoing research effort at Los Alamos National Laboratory (LANL) to learn more about the Earth's radiofrequency (RF) background utilizing satellite-based RF observations of terrestrial lightning. Arguably the richest satellite lightning database ever recorded is that from the Fast On-orbit Recording of Transient Events (FORTE) satellite, which returned at least five years of data from its two RF payloads after launch in 1997. While some classification work has been done previously on the LANL FORTE RF database, application of modern pattern recognition techniques may further lightning research in the scientific community and potentially improve on-orbit processing and event discrimination capabilities for future satellite payloads. We now develop and implement new event classification capability on the FORTE database using state-of-the-art adaptive signal processing combined with compressive sensing and machine learning techniques. The focus of our work is improved feature extraction using sparse representations in learned dictionaries. Extracting classification features from RF signals typically relies on knowledge of the application domain in order to find feature vectors unique to a signal class and robust against background noise. Conventional localized data representations for RF transients using analytical dictionaries, such as a short-time Fourier basis or wavelets, can be suitable for analyzing some types of signals, but not others. Instead, we learn RF dictionaries directly from data, without relying on analytical constraints or additional knowledge about the signal characteristics, using several established machine learning algorithms. Sparse classification features are extracted via matching pursuit search over the learned dictionaries, and used in conjunction with a statistical classifier to distinguish between lightning types. We present preliminary results of our work and discuss classification performance and future development.